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Thermophoresis of water droplets inside carbon nanotubes[1] HARVEY ZAMBRANO, University of Concepcion, JH WALTHER[2], Technical University of Denmark, ELTON OYARZUA, ANDRES ROJANO, University of Concepcion — Carbon Nanotubes (CNTs) offer unique possibilities as fluid conduits with applications ranging from lab on a chip devices to encapsulation media for drug delivery. CNTs feature high mechanical strength, chemical and thermal stability and biocompatibility therefore they are promising candidates for nanodevice fabrication. Thermal gradients have been proposed as mechanism to drive particles, fullerenes and droplets inside CNTs. Here, by conducting Molecular Dynamics (MD) simulations, we study thermophoresis of water droplets inside CNTs. We systematically change the size of the droplets, the axial thermal gradient and CNT chirality. We find that the droplet motion in the armchair CNTs exhibits two clearly delimited stages, a regime wherein the droplet is accelerated and subsequently, a regime wherein the droplet moves with constant velocity. Inside the zig zag CNTs, the droplet accelerates during a very short time and then it moves with constant velocity. We compute the net force during the droplet acceleration and find a correlation between the droplet acceleration and the magnitude of the thermal gradient without any dependence on the droplet size. Moreover, we conduct velocity constrained MD simulations to determine the friction and thermophoretic forces acting on the droplet.

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